

WE CLAIM:

1. A method of identifying suitable polymer attachment sites on a protein comprising:
  - a) inputting a three dimensional protein structure with amino acid positions into a computer; and
  - b) analyzing said structure using a simulation module that:
    - i) identifies a set of said positions suitable for attachment of a polymer; and
    - ii) identifies a set of possible polymers;

to generate a matrix of positions and polymers that are energetically favorable.
2. A method according to claim 1 wherein said set of polymers are polymeric conformers.
3. A method according to claim 1 wherein said set of polymers is generated by chain buildup.
4. A method according to claim 1 wherein said set of polymers is generated by utilizing a starting polymeric conformer and perturbing said conformer to generate said set.
5. A method according to claim 4 wherein said perturbation is done using a Monte Carlo search.
6. A method according to claim 4 wherein said perturbation is done using a molecular dynamics method.
7. A method according to claim 1, wherein said protein is a therapeutic protein.
8. A method according to claim 1, wherein said polymer is pharmaceutically acceptable.
9. A method according to claim 1, wherein said polymer is PEG.
10. A method according to claim 1, wherein said polymer has a range of about 1000 daltons to about 100,000 daltons.
11. A method according to claim 1, wherein said polymer is branched.
12. A method according to claim 1, wherein said polymer is unbranched.
13. A method according to claim 1, wherein said polymer is labile.

14. A method according to claim 1, wherein said simulation module includes MC, MD or combinations thereof.
15. A protein with a polymer attachment generated by the method of claim 1.